

Superconducting, Ferromagnetic and Antiferromagnetic Phases in the $t - t'$ Hubbard Model

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We apply a renormalization group approach to the determination of the phase diagram of the $t - t'$ Hubbard model at the Van Hove filling, as function of t'/t , for small values of U/t . The model presents ferromagnetic, antiferromagnetic and d-wave superconducting phases. Antiferromagnetism and d-wave superconductivity arise from the same interactions, and compete in the same region of parameter space.

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In recent years great effort has been devoted to study the role of Van Hove singularities in two-dimensional electron liquids^{1–8}. Most part of the interest stems from the evidence, gathered from photoemission experiments, that the hole-doped copper oxide superconductors tend to develop very flat bands near the Fermi level^{9,10}. The model most widely used for the Cu-O planes is the Hubbard model, which also shows strong antiferromagnetic correlations. The correspondence with the phenomenology of the high- T_c materials is supposed to be attained in the intermediate to strong coupling regime. Weak coupling approaches to the model have shown that it is more likely to develop a spin-density-wave instability than superconductivity near half-filling^{2,3,11}.

The inspection of the actual Fermi line of most of the copper oxide superconductors shows, however, a sensible departure from nesting. In the context of models with on-site interaction, the dispersion relation seems to be best fitted by introducing both nearest neighbor t and next-to-nearest neighbor t' , accomodated in the so-called $t - t'$ Hubbard model¹². In this model, the absence of perfect nesting implies that the antiferromagnetic correlations have a less divergent behavior when the Fermi level lies at the Van Hove singularity. For this reason, it is best suited for the implementation of a renormalization group (RG) approach to the ground state properties, that is needed anyhow to deal with the logarithmic singularities arising from the divergent density of states¹³.

In this Letter we look for the instabilities of the $t - t'$ Hubbard model, filled up to the level of the Van Hove singularity, following the wilsonian RG program of Refs. 14,15. Our approach is that of integrating virtual states of two energy slices above and below the Fermi level in an energy range given by the cutoff E_c , $E_c - |dE_c| < |E| < E_c$. We are interested in the scaling behavior of the interactions and correlations under a progressive reduction of the cutoff, which leads to the description of the low-energy physics about the Fermi level.

In the RG process, we have to make sure first that the interaction does not scale to zero at the classical level, that is, it displays marginal behavior as we approach the Fermi line. When the cutoff is sufficiently close to the Fermi level, as shown in Fig. 1, most part of the states at hand are in the neighborhood of any of the two Van Hove points $(\pi, 0)$ (A) and $(0, \pi)$ (B), and the dispersion relation may be approximated by two respective patches about each of them:

$$\varepsilon_{A,B}(\mathbf{k}) \approx \mp(t \mp 2t')k_x^2a^2 \pm (t \pm 2t')k_y^2a^2 \quad (1)$$

where a is the lattice constant. The angle between the two separatrices is $2 \arctan[(t + 2t')/(t - 2t')]$. The low-energy effective action may be written in the form

$$S = \int d\omega d^2k \sum_{\alpha,\sigma} (\omega a_{\alpha,\sigma}^+(\mathbf{k}, \omega) a_{\alpha,\sigma}(\mathbf{k}, \omega) - \varepsilon_\alpha(\mathbf{k}) a_{\alpha,\sigma}^+(\mathbf{k}, \omega) a_{\alpha,\sigma}(\mathbf{k}, \omega)) \\ - U \int d\omega d^2k \rho_\uparrow(\mathbf{k}, \omega) \rho_\downarrow(-\mathbf{k}, -\omega) \quad (2)$$

where $a_{\alpha,\sigma}(a_{\alpha,\sigma}^+)$ is an electron annihilation (creation) operator (α labels the Van Hove point), $\rho_{\uparrow,\downarrow}$ are the density operators in momentum space, and the momentum integrals are restricted to modes within the energy cutoff, $|\varepsilon_\alpha(\mathbf{k})| \leq E_c$. It is a fact that the action (2) defines a model that is scale invariant at the classical level, that is, the different terms that build up (2) are invariant altogether under a rescaling of the cutoff E_c ⁷. This implies that the interaction in the $t - t'$ Hubbard model has marginal behavior, at least at the classical level, and it is therefore susceptible of a low-energy description within the RG framework.

In our low-energy model, the two patches for the dispersion relation give rise to an additional flavor index. The number of possible interactions proliferates accordingly. The different terms are depicted in Fig. 2. It might seem that the analysis of the quantum corrections in the model should bear a great similarity with the g-ology description of one-dimensional models. In two dimensions, however, kinematical constraints play a crucial role. Performing the wilsonian RG analysis, no singular cutoff dependences are found in the particle-particle channel, for instance, unless the two colliding particles have opposite momenta. This conclusion may be drawn from the general discussion carried out in Ref. 14. The BCS instability is to be analyzed, then, as a singularity in a response function computed at a definite value of the momentum. On the other hand, singular dependences on the cutoff are found in the particle-hole channel, when the momentum transfer is about zero or about the momentum connecting the two Van Hove points, $\mathbf{Q} \equiv (\pi, \pi)$.

The interactions shown in Fig. 2 are renormalized by the high-energy modes at the quantum level. In all the four cases, the only contribution to second order in perturbation theory which is $\sim dE_c/E_c$ is given by a diagram of the type shown in Fig. 3. As mentioned before, the contributions in the particle-particle channel are $O((dE_c)^2)$ for generic values of the incoming and outgoing momenta, and there are no more diagrams which can be built up from the interaction in (2). To second order we get the RG flow equations

$$E_c \frac{\partial U_{intras}}{\partial E_c} = \frac{1}{2\pi^2 t} c (U_{intras}^2 + U_{back}^2) \quad (3)$$

$$E_c \frac{\partial U_{back}}{\partial E_c} = \frac{1}{\pi^2 t} c (U_{intras} U_{back}) \quad (4)$$

$$E_c \frac{\partial U_{inters}}{\partial E_c} = \frac{1}{2\pi^2 t} c' (U_{inters}^2 + U_{umk}^2) \quad (5)$$

$$E_c \frac{\partial U_{umk}}{\partial E_c} = \frac{1}{\pi^2 t} c' (U_{inters} U_{umk}) \quad (6)$$

where $c \equiv 1/\sqrt{1 - 4(t'/t)^2}$ and $c' \equiv \log \left[\left(1 + \sqrt{1 - 4(t'/t)^2} \right) / (2t'/t) \right]$ are the prefactors of the polarizabilities at zero and \mathbf{Q} momentum transfer, respectively.

The RG equations (3)-(6) describe a flow that drives the couplings to large values, as the cutoff is sent to the Fermi line. This is due to the localization in space of the interactions, which makes them strongly spin-dependent. The RG flow of extended, spin-independent, interactions is towards lower couplings, as discussed in Ref. 7. In that case, RPA-like screening is the dominant effect. The limit of a short range interaction is special in that there is a cancellation between the ‘particle-hole bubble’ and ‘vertex-correction’ second order diagrams. For a purely local interaction like that of the $t - t'$ Hubbard model, the only contribution left corresponds to the antiscreening diagram shown in Fig. 3.

In order to apply the above RG equations to the $t - t'$ model, we compute the flow starting with all the couplings set to the original value U of the on-site interaction. Under this initial condition, it is clear that $U_{intras} = U_{back}$ and $U_{inters} = U_{umk}$, all along the flow. The renormalized vertices show divergences at certain values of the frequency, measured in units of the cutoff E_c . We have

$$U_{intras} = \frac{U}{1 + U c / (\pi^2 t) \log(\omega/E_c)} \quad (7)$$

$$U_{inters} = \frac{U}{1 + U c' / (\pi^2 t) \log(\omega/E_c)} \quad (8)$$

We interpret the divergences of the vertices in the same way as in the RPA, as signalling the development of an ordered phase in the system.

The precise determination of the instability which dominates for given values of U and t' is accomplished by analyzing the response functions of the system. The procedure is similar to that followed in the study of one-dimensional electron systems¹⁶. We adopt again a RG approach to their computation, which takes into account the scaling behavior of the interactions (7) and (8). We analyze ferromagnetic, antiferromagnetic, superconducting and CDW correlations. We assume that the actual instabilities of the model at low temperatures are some of these.

It is easily seen that the operators related to charge-density-wave and s-wave superconducting instabilities do not develop divergent correlations at small ω . The phase diagram in the $t' - U$ plane is drawn by looking at the competition among ferromagnetic, antiferromagnetic and d-wave superconducting instabilities. The ferromagnetic response function R_{FM} , for instance, is given by the correlation of the uniform magnetization, $\rho_\uparrow(0, \omega) - \rho_\downarrow(0, \omega)$. The first perturbative terms for this object are built from a couple of one-loop particle-hole diagrams linked by the interaction. Each particle-hole bubble has a logarithmic dependence on the cutoff E_c , with the prefactor $c =$

$1/\sqrt{1 - 4(t'/t)^2}$. The iteration of bubbles can be taken into account by differentiating with respect to E_c and writing a self-consistent equation for R_{FM} , which turns out to be

$$\frac{\partial R_{FM}}{\partial E_c} = -\frac{2c}{\pi^2 t} \frac{1}{E_c} + \frac{c}{\pi^2 t} (U_{intras} + U_{inters}) \frac{1}{E_c} R_{FM} \quad (9)$$

The antiferromagnetic response function R_{AFM} can be dealt with in a similar fashion, by looking at correlations of the operator $\rho_\uparrow(\mathbf{Q}, \omega) - \rho_\downarrow(\mathbf{Q}, \omega)$. This leads to the RG equation

$$\frac{\partial R_{AFM}}{\partial E_c} = -\frac{2c'}{\pi^2 t} \frac{1}{E_c} + \frac{c'}{\pi^2 t} (U_{back} + U_{umk}) \frac{1}{E_c} R_{AFM} \quad (10)$$

We recall that $U_{intras} + U_{inters}$ and $U_{back} + U_{umk}$ have the same flow, within the present model. Therefore, we may discern at once that whenever $c > c'$ the ferromagnetic response function R_{FM} prevails over R_{AFM} .

Finally, there remains the response function for d-wave superconductivity R_{SCd} , which is given by the correlation of the operator $\sum_{\mathbf{k}} (a_{A\uparrow}^+(\mathbf{k}) a_{A\downarrow}^+(-\mathbf{k}) - a_{B\uparrow}^+(\mathbf{k}) a_{B\downarrow}^+(-\mathbf{k}) + h.c.)$. The computation within the RG framework becomes now a little bit more subtle, since the diagrams at strictly zero total momentum display a $\log^2 E_c$ dependence on the cutoff. As the derivative with respect to E_c is taken, it becomes clear that the logarithmic dependence left corresponds to the divergent density of states at the Van Hove singularity. The RG equation for R_{SCd} reads then

$$\frac{\partial R_{SCd}}{\partial E_c} = -\frac{c}{2\pi^2 t} \frac{\log(E_c/\omega)}{E_c} - \frac{c}{2\pi^2 t} (U_{intras} - U_{umk}) \frac{\log(E_c/\omega)}{E_c} R_{SCd} \quad (11)$$

This equation also shows an homogeneous scaling of R_{SCd} on ω/E_c , like in the previous cases.

From inspection of Eq. (11), it is clear that divergent correlations in the d-wave channel arise for $U_{intras} - U_{umk} < 0$. According to the above results, this only happens for $c < c'$, that is, outside the region of the phase diagram where $R_{FM} > R_{AFM}$. This confirms that a ferromagnetic regime sets in for values of t' above the critical value $t'_c \approx 0.276t$ at which $c = c'$. For values below t'_c , there is a competition between R_{AFM} and R_{SCd} , which requires the analysis of the respective behaviors close to the critical frequency at which the response functions diverge. As a general trend, the response function R_{SCd} dominates over R_{AFM} in the regime of weak interaction, the strength being measured with regard to both the bare coupling constant and the value of the c' parameter. The reason for such behavior is that at weak interaction strength the RG flow has a longer run to reach the critical frequency, and at small frequencies the logarithmic density of states in Eq. (11) makes R_{SCd} to grow larger. The border where the crossover between the antiferromagnetic and the superconducting instability takes place is shown in the $t' - U$ phase diagram of Fig. 4. At sufficiently large values of U and small values of t' , the leading instability of the system turns out to be antiferromagnetism. This is in agreement with weak coupling RG analyses applied to the Hubbard model^{2,3,11}.

Thus, there exists a region of the phase diagram where superconductivity is the leading instability. We remark that this result is obtained within a RG approach that provides a rigorous computational framework, with no other assumption than the weakness of the bare interaction. The instabilities are led by an unstable RG flow, and the singular behavior of the response functions is interpreted in the same fashion than in a standard RPA computation. The wide range for superconductivity is consistent with the results from quantum Monte Carlo computations¹⁷, as well as with results obtained by exact diagonalization of small clusters in the strong coupling regime¹⁸.

On the other hand, the renormalized interactions remain most part of the flow in the weak coupling regime for $U/t < 1$. We observe that the most interesting region in the phase diagram of Fig. 4 starts near $U/t \approx 1$, where the critical frequencies are $\omega_c \sim 10^{-2} E_c$. This order of magnitude corresponds to sizeable critical temperatures (~ 100 K) if we assign to E_c a value of the order of the conduction bandwidth in the cuprates (~ 1 eV).

The other relevant conclusion within our RG approach is the existence of a ferromagnetic regime in the $t - t'$ model, above a certain value of the t' parameter. This is consistent with the results obtained in Ref. 19 close to $t' = 0.5t$. Though our results refer to the weak coupling regime, they show that antiferromagnetic, ferromagnetic and superconducting phases are all realized in the $t - t'$ Hubbard model. The superconducting instability has greater strength at the boundary with the antiferromagnetic instability, as it also happens in other approaches to high- T_c superconductivity²⁰.

In our case, the diagrams responsible for the appearance of superconductivity cannot be interpreted in terms of the exchange of antiferromagnetic fluctuations, as in the work mentioned earlier²⁰. Those diagrams which contain bubbles mediating an effective interaction between electron propagators are cancelled, to all orders, by vertex corrections (see Fig. 3). Superconductivity arises from the type of diagrams first studied by Kohn and Luttinger²¹. The strong anisotropy of the Fermi surface greatly enhances the Kohn-Luttinger mechanism, with respect to its effect in an isotropic metal⁷.

Our results support the idea that d-wave superconductivity and antiferromagnetism arise from the same type of interactions. Antiferromagnetism, however, does not favor the existence of superconductivity, but competes with it in the same region of parameter space. Similar physical processes seem to be responsible for the appearance of anisotropic superconductivity in systems of coupled repulsive 1D chains²². The Fermi surface of a single chain is unable to give rise to this type of superconductivity. As soon as this limitation is lifted, superconductivity occupies a large fraction of the phase diagram previously dominated by antiferromagnetic fluctuations.

The results reported above can be extended to fillings away from the Van Hove singularity, provided that the distance of the chemical potential to the singularity is smaller than the energy scale at which the instability takes place. The chemical potential tends to be pinned to the singularity because of the nontrivial RG flow of the chemical potential itself⁷. Hence, these calculations can be applied to a finite range of fillings around that appropriate to the singularity.

In conclusion, we have shown that the $t - t'$ Hubbard model at the Van Hove singularity exhibits a variety of instabilities at low energies or temperatures. The existence of these instabilities can be derived by RG methods which become exact at small couplings. We find that antiferromagnetism and d-wave superconductivity arise from the same interactions, and compete with each other in the same region of parameter space.

- ¹ J. Labbé and J. Bok, *Europhys. Lett.* **3**, 1225 (1987); J. Friedel, *J. Phys. (Paris)* **48**, 1787 (1987); *ibid.* **49**, 1435 (1988).
- ² H. J. Schulz, *Europhys. Lett.* **4**, 51 (1987).
- ³ J. E. Dzyaloshinskii, *Pis'ma Zh. Eksp. Teor. Fiz.* **46**, 97 (1987) [JETP Lett. **46**, 118 (1987)].
- ⁴ P. A. Lee and N. Read, *Phys. Rev. Lett.* **58**, 2691 (1988).
- ⁵ R. S. Markiewicz, *J. Phys. Condens. Matter* **2**, 665 (1990); R. S. Markiewicz and B. G. Giessen, *Physica (Amsterdam)* **160C**, 497 (1989).
- ⁶ C. C. Tsuei *et al.*, *Phys. Rev. Lett.* **65**, 2724 (1990); P. C. Pattnaik *et al.*, *Phys. Rev. B* **45**, 5714 (1992).
- ⁷ J. González, F. Guinea and M. A. H. Vozmediano, *Europhys. Lett.* **34**, 711 (1996); *Nucl. Phys. B* **485**, 694 (1997).
- ⁸ L. B. Ioffe and A. J. Millis, *Phys. Rev. B* **54**, 3645 (1996).
- ⁹ Z.-X. Shen *et al.*, *Science* **267**, 343 (1995), and references therein.
- ¹⁰ K. Gofron *et al.*, *Phys. Rev. Lett.* **73**, 3302 (1994).
- ¹¹ D. Zanchi and H. J. Schulz, *Phys. Rev. B* **54**, 9509 (1996).
- ¹² P. Bénard, L. Chen and A. M. Tremblay, *Phys. Rev. B* **47**, 15217 (1993); Q. Si, T. Zha, K. Levin and J. P. Lu, *ibid.* **47**, 9055 (1993); A. Nazarenko *et al.*, *ibid.* **51**, 8676 (1995); D. Duffy and A. Moreo, *ibid.* **52**, 15607 (1995); A. F. Veilleux *et al.*, *ibid.* **52**, 16255 (1995).
- ¹³ H. Q. Lin and J. E. Hirsch, *Phys. Rev. B* **35**, 3359 (1987).
- ¹⁴ R. Shankar, *Rev. Mod. Phys.* **66**, 129 (1994).
- ¹⁵ J. Polchinski, in *Proceedings of the 1992 TASI in Elementary Particle Physics*, J. Harvey and J. Polchinski eds. (World Scientific, Singapore, 1992).
- ¹⁶ J. González, M. A. Martín-Delgado, G. Sierra and M. A. H. Vozmediano, *Quantum Electron Liquids and High-T_c Superconductivity* (Springer-Verlag, Berlin, 1995).
- ¹⁷ T. Husslein *et al.*, *Phys. Rev. B* **54**, 16179 (1996).
- ¹⁸ J. González and J. V. Alvarez, preprint (cond-mat/9609162), to be published in *Phys. Rev. B*.
- ¹⁹ S. Sorella, R. Hlubina and F. Guinea, *Phys. Rev. Lett.* **78**, 1343 (1997).
- ²⁰ N. E. Bickers, D. J. Scalapino and S. R. White, *Phys. Rev. Lett.* **62**, 961 (1989); E. Dagotto, J. Riera and A. P. Young, *Phys. Rev. B* **42**, 2347 (1990); P. Monthoux and D. Pines, *Phys. Rev. Lett.* **69**, 961 (1992); E. Dagotto and J. Riera, *ibid.* **70**, 682 (1993); E. Dagotto, A. Nazarenko and A. Moreo, *ibid.* **74**, 310 (1995). K. Maki and H. Won, *Phys. Rev. Lett.* **72**, 1758 (1994).
- ²¹ W. Kohn and J. M. Luttinger, *Phys. Rev. Lett.* **15**, 524 (1965).
- ²² H.-H. Lin, L. Balents and M. P. A. Fisher, preprint (cond-mat/9703055).

FIG. 1. Energy contour lines about the Fermi level, with the Fermi line passing by the saddle points A and B.

FIG. 2. Different interaction terms arising from the flavor indexes A and B.

FIG. 3. Second order diagram renormalizing the different interactions in the model, with electron lines carrying flavor index A or B appropriate to each case.

FIG. 4. Phase diagram in the (t', U) plane. The dotted lines are contour lines corresponding to the critical frequencies shown in the figure.







